

## Propofol - Compound Summary (CID 4943)



### » Structure & Quick Link Bar

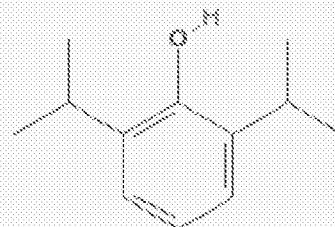
2D

3D

An intravenous anesthetic agent which has the advantage of a very rapid onset after infusion or bolus injection plus a very short recovery period of a couple of minutes. (From Smith and Reynard, Textbook of Pharmacology, 1992, 1st ed, p206). Propofol has been used as ANTICONVULSANTS and ANTIEMETICS.◆

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[⇒ PC3D Viewer Download](#)

Compound ID	4943	🔗
Molecular Weight	178.27072 [g/mol]	🔗
Molecular Formula	C <sub>12</sub> H <sub>18</sub> O	🔗
XLogP3	3.8	🔗
H-Bond Donor	1	🔗
H-Bond Acceptor	1	🔗



BioMedical Annotation: (Total:1) 🔗



### Propofol

#### Medication Information 🔗

##### ◆ Diprivan [General Injectables & Vaccines, Inc]

For IV Administration OnlyRx OnlyStrict aseptic technique must always be maintained during handling. Diprivan Injectable Emulsion is a single-use parenteral product which contains 0.005% disodium edetate to inhibit the rate of growth of [more...](#)

Description	Clinical Pharmacology	Indication & Usage
Contraindications	Warnings	Precautions
Adverse Reactions	Overdosage	Dosage & Administration
How Supplied		

##### ◆ Diprivan Injectable Emulsion, USP [APP

### Links

Protein Structure (3) 🔗  
 PubMed (29) 🔗  
 Gene (389) 🔗  
 Taxonomy (5) 🔗  
 NLM Toxicology Link 🔗

Chemical Structure Search 🔗  
 BioActivity Summary: 🔗  
 This Compound  
 with Similar Compounds

Related Compounds: 🔗  
 Same, Connectivity: 4 Links

Similar Compounds: 2137 Links 🔗  
 Similar Conformers: 1267 Links  
[View Conformers](#) 🔗

Substances: 🔗  
 All: 189 Links  
 Same structure: 77 Links

## EXHIBIT B

Pharmaceuticals, LLC]

Mixture: 112 Links

⊗ **Diprivan Injectable Emulstion, USP** [APP Pharmaceuticals, LLC]

⊗ **DIPRIVAN** [AstraZeneca Pharmaceuticals LP]

⊗ **PROPOFOL INJECTABLE EMULSION 1%** [Bedford Laboratories]

⊗ **PROPOFOL Injectable Emulsion 1%** [Hospira, Inc.]

⊗ **Propofol Injectable Emulsion 1%** [Teva Parenteral Medicines, Inc.]

⊗ **Propofol Injectable Emulsion, USP** [APP Pharmaceuticals, LLC]

⊗ **Propofol Injectable Emulsion, USP** [APP Pharmaceuticals, LLC]

⊗ **Propofol Injectable Emulsion, USP** [APP Pharmaceuticals, LLC]

⊗ **Propofol Injectable Emulsion, USP** [APP Pharmaceuticals, LLC]

### Pharmacological Action

Hypnotics and Sedatives ⊗ - Drugs used to induce drowsiness or sleep or to reduce psychological excitement or anxiety.

Anesthetics, Intravenous ⊗ - Ultrashort-acting anesthetics that are used for induction. Loss of consciousness is rapid and induction is pleasant, but there is no muscle ... ⊗

### ⊗ Pharmacological Classification

Chemical Actions and Uses⊗

Pharmacologic Actions⊗

Physiological Effects of Drugs⊗

Central Nervous System Depressants⊗

Anesthetics⊗

Anesthetics, General⊗

**Anesthetics, Intravenous⊗**

**Hypnotics and Sedatives⊗**

**Hypnotics and Sedatives⊗**

Therapeutic Uses⊗

Central Nervous System Agents⊗

Central Nervous System Depressants⊗

Anesthetics⊗

Anesthetics, General⊗

**Anesthetics, Intravenous⊗**

**Hypnotics and Sedatives⊗**

**Hypnotics and Sedatives⊗**

**Chemical Classification**

Organic Chemicals

Phenols

Propofol

**Safety and Toxicology**

HSDB - Peer-reviewed summary of toxicity and biomedical effects

CCRIS - Carcinogenicity, tumor promotion, tumor inhibition, and mutagenicity tests

EINECS - European Inventory of Existing Commercial Chemical Substances

TOXLINE - Citations to the toxicological literature

LactMed - Information on chemicals that breastfeeding mothers may be exposed

ClinicalTrials.gov - Registry of federal and private clinical trials

**Literature** Choose by Subheadings:

administration and dosage	adverse effects	agonists
analogues and derivatives	analysis	antagonists and inhibitors
blood	cerebrospinal fluid	chemical synthesis
chemistry	classification	contraindications
diagnostic use	economics	history
immunology	isolation and purification	metabolism
pharmacokinetics	pharmacology	poisoning
standards	supply and distribution	therapeutic use
toxicity	urine	

**Literature Keyword Mining Tool****BioAssay Results:**

Tested in BioAssays: All: 447 Active: 6 Inactive: 364  
 BioActivity Summary: This Compound with Similar Compounds

## EXHIBIT B

**AID:** 119873 **Source:** ChEMBL **DataTable**

Speed of induction of analgesia in mice was determined;  
I = immediate, <10 s

**AID:** 109886 **Source:** ChEMBL **DataTable**

Duration of analgesic action in mice was determined; B  
= brief, < 5 min

**AID:** 1195 **Source:** EPA DSSTox **DataTable**

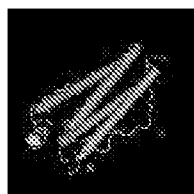
DSSTox (FDAMDD) FDA Maximum (Recommended) Daily  
Dose Database

**AID:** 590 **Source:** NCGC **DataTable**

qHTS Assay for Spectroscopic Profiling in A350 Spectral  
Region

more ...

### Protein Structures: (Total: 2)



**MMDB ID:** 75300 **PDB ID:** 3F33

Apoferritin: Complex With Propofol

**Taxonomy:** Equus caballus









**MMDB ID:** 15377 **PDB ID:** 1E7A

Crystal Structure Of Human Serum  
Albumin Complexed With The General  
Anesthetic Propofol

**Taxonomy:** Homo sapiens

### Depositor-Supplied Synonyms: (Total: 126)

Display: Next 10 | All | Sort: **Weight**

propofol   
Diprivan   
Disoprofol   
Disoprivan   
Diisopropylphenol  
2,6-DIISOPROPYLPHENOL   
Propofolum  
Dipravan  
Fresofol   
Rapinovet

### Properties Computed from Structure:

Molecular Weight	178.27072 [g/mol]
Molecular Formula	C <sub>12</sub> H <sub>18</sub> O
XLogP3	3.8
H-Bond Donor	1

## EXHIBIT B

H-Bond Acceptor	1
Rotatable Bond Count	2
Tautomer Count	2
Exact Mass	178.135765
Monoisotopic Mass	178.135765
Topological Polar Surface Area	20.2
Heavy Atom Count	13
Formal Charge	0
Complexity	135
Isotope Atom Count	0
Defined Atom StereoCenter Count	0
Undefined Atom StereoCenter Count	0
Defined Bond StereoCenter Count	0
Undefined Bond StereoCenter Count	0
Covalently-Bonded Unit Count	1



### Descriptors Computed from Structure: ⓘ



**IUPAC Name:** 2,6-di(propan-2-yl)phenol  
**Canonical SMILES:** CC(C)C1=C(C(=CC=C1)C(C)C)O  
**InChI:** InChI=1S/C12H18O  
/c1-8(2)10-6-5-7-11(9(3)4)12(10)13/h5-9,13H,1-4H3  
**InChIKey:** OLBCVFGFOZPWHH-UHFFFAOYSA-N ⓘ



### Compound Information: ⓘ



**CID** 4943 ⓘ ⓘ

Create Date: 2005-03-25

**Related Compounds:** ⓘ

Same, Connectivity: 4 Links

**Similar Compounds:** 2137 Links ⓘ

**Similar Conformers:** 1267 Links View Conformers ⓘ



### Substance Information: ⓘ



**Substances:** ⓘ

All: 189 Links

Same structure: 77 Links

Mixture: 112 Links

**Category:** [for same structure substances] ⓘ

Biological Properties: 32 Links

BIDD ( 1 )

SID 93166594 - External ID: BIDD:GT0436

ChEBI ( 1 )

SID 26697200 - External ID: CHEBI:44915

ChemBank ( 10 ) ⓘ

ChemSpider ( 6 ) ⓘ

Circadian Research, Kay Laboratory, University of California at San Diego (UCSD) ( 1 )

SID 92303746 - External ID: D126608

Comparative Toxicogenomics Database ( 1 )

## EXHIBIT B

SID 53788803 - External ID: D015742  
DiscoveryGate ( 1 )  
SID 8153049 - External ID: 4943  
DrugBank ( 1 )  
SID 46504991 - External ID: DB00818  
DTP/NCI ( 1 )  
SID 71265 - External ID: 5105  
ICCB-Longwood/NSRB Screening Facility, Harvard  
Medical School ( 3 )  
SID 92125828 - External ID: HMS1570L04  
SID 92308977 - External ID: HMS2089O21  
SID 92308180 - External ID: HMS2094E17  
LeadScope ( 1 )  
SID 49855158 - External ID: LS-996  
NextBio ( 1 )  
SID 80426669 - External ID: 4943  
NIAID ( 1 )  
SID 219945 - External ID: 123996  
NovoSeek ( 1 )  
SID 57322542 - External ID: 4943  
Southern Research Institute ( 1 )  
SID 49699215 - External ID: AB00513968  
xPharm ( 1 )  
SID 7980416 - External ID: 9305

Chemical Reactions: 8 Links  
ChemSpider ( 6 ) ⓘ  
Comparative Toxicogenomics Database ( 1 )  
SID 53788803 - External ID: D015742  
KUMGM ( 1 )  
SID 7984535 - External ID: ghl.PD\_Mitscher\_leg0.558

Journal Publishers: 2 Links  
Prous Science Drugs of the Future ( 1 )  
SID 12012653 - External ID: 90057  
Thomson Pharma ( 1 )  
SID 14772701 - External ID: 00003209

Metabolic Pathways: 4 Links  
BioCyc ( 1 )  
SID 85256986 - External ID: CPD-11437  
Comparative Toxicogenomics Database ( 1 )  
SID 53788803 - External ID: D015742  
KEGG ( 2 )  
SID 9726 - External ID: C07523  
SID 7847615 - External ID: D00549

NIH Molecular Libraries: 14 Links  
Broad Institute ( 1 )  
SID 85788322 - External ID: BRD-K82255054-001-03-5  
Emory University Molecular Libraries Screening Center  
( 2 )  
SID 17405000 - External ID: EU-0100437  
SID 26612728 - External ID: SPECTRUM1505022  
NCGC ( 10 ) ⓘ  
University of Pittsburgh Molecular Library Screening  
Center ( 1 )  
SID 53777543 - External ID: 391

NIH Substance Repository: 2 Links

## EXHIBIT B

### MLSMR ( 2 )

SID 47193694 - External ID: MLS001066348

SID 85148728 - External ID: MLS002454360

### Physical Properties: 13 Links

#### ChemExper Chemical Directory ( 1 )

SID 3132933 - External ID: HkIH@@RYfVya`Hbj@@@

#### ChemSpider ( 6 )

#### DrugBank ( 1 )

SID 46504991 - External ID: DB00818

#### MP Biomedicals ( 2 )

SID 85088964 - External ID: 193707

SID 51074363 - External ID: 204044

#### NIST ( 1 )

SID 10427917 - External ID: 1803667406

#### NIST Chemistry WebBook ( 1 )

SID 10513227 - External ID: 1803667406

#### NMRShiftDB ( 1 )

SID 8001758 - External ID: 20040435

### Protein 3D Structures: 3 Links

#### MMDB ( 2 )

SID 838001 - External ID: 15377.3

SID 81087128 - External ID: 75300.8

#### SMID ( 1 )

SID 7889810 - External ID: PFL

### Substance Vendors: 13 Links

#### Ambinter ( 1 )

SID 48505627 - External ID: ST5405911

#### ChemExper Chemical Directory ( 1 )

SID 3132933 - External ID: HkIH@@RYfVya`Hbj@@@

#### ChemSynthesis ( 1 )

SID 56289300 - External ID: 19324

#### Hangzhou APiChem Technology ( 1 )

SID 92716688 - External ID: AC-2038

#### IS Chemical Technology ( 1 )

SID 81042045 - External ID: S01-0189

#### Jamson Pharmachem Technology ( 1 )

SID 96022658 - External ID: Jsp004266

#### MolPort ( 1 )

SID 88837501 - External ID: MolPort-001-794-517

#### MP Biomedicals ( 2 )

SID 85088964 - External ID: 193707

SID 51074363 - External ID: 204044

#### Sigma-Aldrich ( 2 )

SID 24278001 - External ID: D126608\_ALDRICH

SID 24902022 - External ID: W505102\_ALDRICH

#### TCI (Tokyo Chemical Industry) ( 1 )

SID 87567266 - External ID: D0617

#### ZINC ( 1 )

SID 12055958 - External ID: ZINC00968303

### Theoretical Properties: 9 Links

#### ChemDB ( 1 )

SID 5371511 - External ID: 3968273

#### ChemSpider ( 6 )

#### DrugBank ( 1 )

SID 46504991 - External ID: DB00818

#### ZINC ( 1 )

## EXHIBIT B

SID 12055958 - External ID: ZINC00968303

Toxicology: 4 Links

ChemIDplus ( 1 )

SID 159631 - External ID: 002078548

Comparative Toxicogenomics Database ( 1 )

SID 53788803 - External ID: D015742

EPA DSSTox ( 2 )

SID 48416482 - External ID: 23523

SID 48424532 - External ID: 32895

ASN1

XML

SDF

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